Computing Linear Combinations of φ Functions

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We consider the time integration of large stiff systems of ordinary differential equations, which result from semidiscretization of partial differential equations and are of the form

$$u'(t) = Au(t) + g(u(t)), \quad u(0) = u_0. \tag{1}$$

We introduce a class of numerical methods for the time integration of these problems, the so-called exponential integrators, and discuss the construction and analysis of these methods using the Volterra integral equation which gives the exact solution for (1).

When implementing exponential integrators one needs to evaluate the action of matrix functions (e.g. matrix exponential) on vectors. We consider using Krylov subspace methods for these problems, and introduce a so-called moment-matching Arnoldi iteration for computing sums of the form

$$\exp(hA)w_0 + \sum_{k=1}^{p} h^k \varphi_k(hA) w_k,$$

a where $A \in \mathbb{C}^{n \times n}$, $w_i \in \mathbb{C}^n$, $1 \leq i \leq p$, $h \in \mathbb{R}$, and the functions φ_k are closely related to the exponential function. We show how to obtain a priori error bounds for the error of the moment-matching approximation using Cauchy's integral formula, and how to derive a posteriori error estimates.

One particular example for exponential integrators and φ functions comes from classical electromagnetism. We consider the equations of motion for a single particle given by

$$\begin{aligned} \frac{d}{dt} q &= p/m, \\ \frac{d}{dt} p &= E(q) + \Omega(q)p, \end{aligned}$$

where $E(q)$ represents an external electric field, and $\Omega(q)$ is a skew-symmetric 3×3 matrix representing the Lorentz forces from an external magnetic field. Here, $\exp(h\Omega)$ and the φ functions are easily computed with the help of the Rodrigues' formula. By using splitting strategies one can construct integrators that preserve well the structure of the equation (Hamiltonian structure, time symmetry, volume, energy).